At a Glance

Transport Monte Carlo simulation of conduction in biological Ionic Channels.

Description

The BioMOCA code has progressed steadily to become a flexible tool for investigation of ionic transport that can be used as a complement of more expensive Molecular Dynamics simulations. This picture shows results from a simulation of ompf porin ionic channel. The volumes occupied by traversal trajectories followed by a K+ ion (green) and a Cl− ion (grey) show how cation and anion occupy different portion of the pore, reflecting the highly charge nature of the protein forming the channel. Available Molecular Dynamics simulations can only give a hint of such behavior, since time-resolution is restricted by computational cost. The information is very valuable for the analysis of pioneering devices that incorporate membranes with porin channels. A prototype device has been realized recently, for instance, at Arizona State University. Nugget for NCN Annual Report provided by Umberto Ravaioli of UIUC.

Related Documents and Links

- First Time User's Guide

Credits

Computational Electronics Group, University of Illinois at Urbana-Champaign.
First Time User's Guide

Running Your First MOSCV Simulation
This is a step-by-step guide to running BioMOCA in the simulation hub.

**Note:** BioMOCA uses input files to set the physical and numerical parameters, and needs the protein structure (PDB or PQR files.) However in this demo version of BioMOCA you do not need to have the head ache of dealing with all the hastles regarding setting up a simulation. Instead you may choose some prestructured protein channels and then adjust a few of the physica and numerical parameters and simply run the code. The output here is just the 2D snapshot visualization of the ion densities and potential. Runnig BioMOCA to get statistical data (ionic permeation) requires long periods of running and working with other more sophisticated output files. Perhaps that would be available to more professional users who may want to get the source code and work with them.

**Step by Step Procedure**

1) On the first tab “Ion Channel” you may have two options of channels, i.e. Gramicidin channel and Porin. Bellow that are the type of solutes with the relative densities on either side of the channel.
2) “Run Parameters” tab determines some of the numerical parameters like the potential across the channel, and the length of simulation in nano seconds and time steps.
3) Gramicidin channel needs a lot longer simulations as the pore is very narrow. However Porin, though it has a much larger structure, the simulation time could be quite shorter as here we have three pores instead of one!
4) Next on the output section there are 24 snapshots of the channel (12 alonge the channel and 12 acroos the channel.)
5) At the end of “Output Log” section we have a brief summery of some statistical data regarding the trace of ions
   - note that the last two lines have some information regarding the number of ions crossed the channel from Left to Right or the other way.
   - These data are sorted in 16 columns of integers:
     - the first two columns indicate the number of cations, and anions respectively.
     For instance: “# crossing R->L 3 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0” means that 3 cations (i.e. Na ions) have crossed from Right bath to the Left bath and also 1 anion (i.e. Cl) ion has crossed the channel...